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(FILE 'HOME' ENTERED AT 11:04:01 ON 08 JUL 2004)

FILE 'REGISTRY' ENTERED AT 11:05:19 ON 08 JUL 2004

L1            1 S NICARDIPIINE/CN  
L2            1 S NIFEDIPIINE/CN

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L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 21829-25-4 REGISTRY  
CN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(2-nitrophenyl)-  
, dimethyl ester (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(o-nitrophenyl)-  
, dimethyl ester (8CI)  
OTHER NAMES:  
CN 2,6-Dimethyl-3,5-dicarbomethoxy-4-(2-nitrophenyl)-1,4-dihdropyridine  
CN 2,6-Dimethyl-4-(2-nitrophenyl)-1,4-dihdropyridine-3,5-dicarboxylic acid  
dimethyl ester  
CN 4-(2-Nitrophenyl)-2,6-dimethyl-3,5-dicarbomethoxy-1,4-dihdropyridine  
CN Adalat  
CN Adalat 10  
CN Adalat 20  
CN Adalat 5  
CN Adalat CC  
CN Adalat CR  
CN Adalat Crono  
CN Adalat FT  
CN Adalat GITS  
CN Adalat GITS 30  
CN Adalat LA  
CN Adalat LP  
CN Adalat Oros  
CN Adalat PA  
CN Adalat Retard  
CN Adalate  
CN Adapine  
CN Adapress  
CN Alat  
CN Aldipin  
CN Alfadat  
CN Alonix  
CN Alonix S  
CN Alpha-Nifedipine Retard  
CN Angipec  
CN Anifed  
CN Anpine  
CN Apo-Nifed  
CN Aprical  
CN BAY 1040  
CN BAY-a 1040  
CN Bonacid  
CN Calcibloc  
CN Calcigard  
CN Calcilat  
CN Camont  
CN Cardifen  
CN Cardilat  
CN Cardilate  
CN Cardionorm  
CN Chronadalate  
CN Chronadalate LP  
CN Citilat  
CN Coracten  
CN Coral  
CN Cordafen

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H donors (HD)	1	(1)	ACD
Koc (KOC)	2.13	pH 1	(1) ACD
Koc (KOC)	587	pH 4	(1) ACD
Koc (KOC)	1090	pH 7	(1) ACD
Koc (KOC)	1091	pH 8	(1) ACD
Koc (KOC)	1091	pH 10	(1) ACD
logD (LOGD)	0.34	pH 1	(1) ACD
logD (LOGD)	2.78	pH 4	(1) ACD
logD (LOGD)	3.05	pH 7	(1) ACD
logD (LOGD)	3.05	pH 8	(1) ACD
logD (LOGD)	3.05	pH 10	(1) ACD
logP (LOGP)	3.054+/-0.590		(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	346.33		(1) ACD
pKa (PKA)	3.93+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	3.37E-09 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.67 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

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CN **Nifedipine**

ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use FCN, FIDE, or ALL for  
DISPLAY

FS 3D CONCORD

DR 11104-22-6, 101539-70-2, 101554-38-5

MF C17 H18 N2 O6

CI COM

LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*,  
BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CBNB,  
CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU,  
DETERM\*, DIOGENES, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH,  
IMSPATENTS, IPA, MEDLINE, MRCK\*, MSDS-OHS, NIOSHTIC, PHAR, PROMT,  
PROUSDDR, PS, RTECS\*, SPECINFO, TOXCENTER, USAN, USPAT2, USPATFULL, VETU  
(\*File contains numerically searchable property data)

Other Sources: DSL\*\*, EINECS\*\*, WHO

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

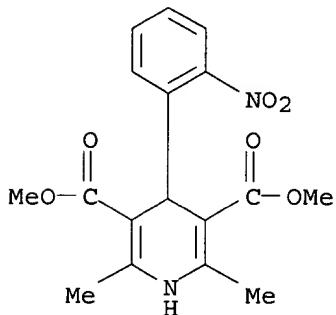
DT.CA Cplus document type: Book; Conference; Dissertation; Journal; Patent;  
Report

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);  
PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or  
reagent); USES (Uses)

RLD.P Roles for non-specific derivatives from patents: ANST (Analytical  
study); BIOL (Biological study); PREP (Preparation); PROC (Process);  
USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological  
study); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC  
(Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical  
study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP  
(Preparation); PROC (Process); PRP (Properties); RACT (Reactant or  
reagent); USES (Uses)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

7031 REFERENCES IN FILE CA (1907 TO DATE)

102 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

7047 REFERENCES IN FILE CAPLUS (1907 TO DATE)

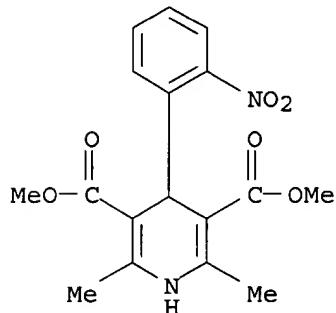
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L2 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

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IN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(2-nitrophenyl)-  
, dimethyl ester (9CI)  
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT  
MF C17 H18 N2 O6  
CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> d prop l2

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

#### Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Melting Point (MP)	172-174 deg C		(1) IC
Melting Point (MP)	172-173 deg C	Solv: methanol	(2) IC (67-56-1)

(1) Cupka, Pavol; CS 243590 B1 1987 CAPLUS

(2) Loev, Bernard; Journal of Medicinal Chemistry 1974 V17(9) P956-65 CAPLUS

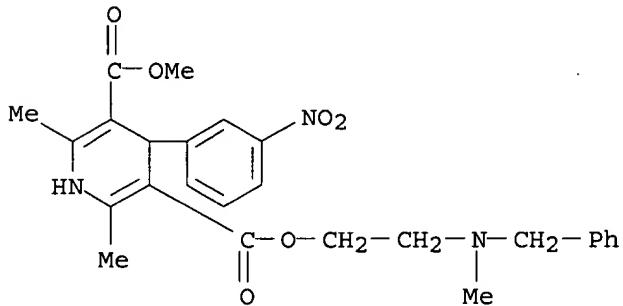
#### Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	66.3	pH 4	(1) ACD
Bioconc. Factor (BCF)	123	pH 7	(1) ACD
Bioconc. Factor (BCF)	123	pH 8	(1) ACD
Bioconc. Factor (BCF)	123	pH 10	(1) ACD
Boiling Point (BP)	475.3+/-45.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	73.87+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	241.2+/-51.7 deg C		(1) ACD
H acceptors (HAC)	8		(1) ACD

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L1 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-  
, methyl 2-[methyl(phenylmethyl)amino]ethyl ester (9CI)  
MF C26 H29 N3 O6  
CI COM

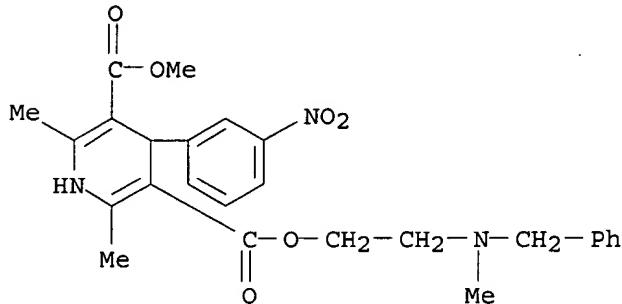


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L1 1 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN  
IN 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-  
, methyl 2-[methyl(phenylmethyl)amino]ethyl ester (9CI)  
MF C26 H29 N3 O6  
CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> d prop

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

#### Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Melting Point (MP)	168.5 deg C	Solv: acetone (67-64-1)	(1) IC

(1) Nakamoto, Yasumasa; JP 62059261 A2 1987 CAPLUS

#### Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	5.04	pH 4	(1) ACD
Bioconc. Factor (BCF)	2395	pH 7	(1) ACD
Bioconc. Factor (BCF)	4841	pH 8	(1) ACD
Bioconc. Factor (BCF)	5454	pH 10	(1) ACD
Boiling Point (BP)	603.4 +/- 55.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	89.75 +/- 3.0 kJ/mol		(1) ACD
Flash Point (FP)	318.7 +/- 56.7 deg C		(1) ACD
H acceptors (HAC)	9		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD

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Koc (KOC)	15.2	pH 4	(1) ACD
Koc (KOC)	7220	pH 7	(1) ACD
Koc (KOC)	14592	pH 8	(1) ACD
Koc (KOC)	16440	pH 10	(1) ACD
logD (LOGD)	0.27	pH 1	(1) ACD
logD (LOGD)	2.19	pH 4	(1) ACD
logD (LOGD)	4.86	pH 7	(1) ACD
logD (LOGD)	5.17	pH 8	(1) ACD
logD (LOGD)	5.22	pH 10	(1) ACD
logP (LOGP)	5.221+/-0.622		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	479.53		(1) ACD
pKa (PKA)	7.11+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	1.63E-14 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.67 ((C) 1994-2004 ACD/Labs)

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